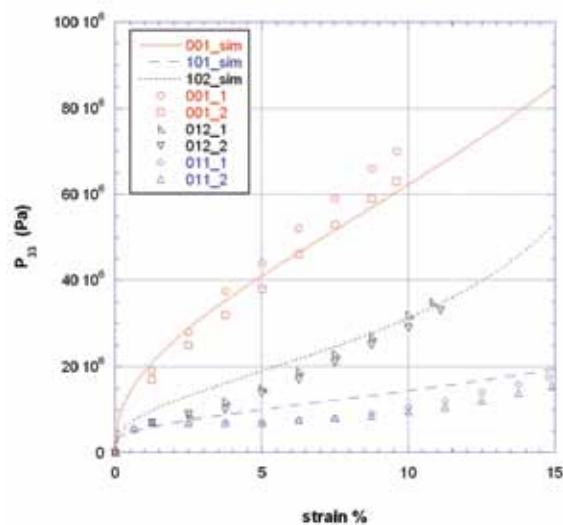


Modeling Metallic Single Crystal Plastic Hardening through the Evolution of Dislocation Subgrain Structure

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Fig. 1. shows a comparison between simulated and experimental stress-strain curves for copper single crystals.



A single crystal plasticity theory was formulated using sequential laminates to model subgrain dislocation structures. It is known that local models do not adequately account for latent hardening, as latent hardening is a nonlocal property as well as a material property (e.g., grain size and shape). The addition of the nonlocal energy from the formation of subgrain structure dislocation walls and the boundary layer misfits provide both latent and self-hardening of crystal slip. Latent hardening occurs as the formation of new dislocation walls limit motion of new mobile dislocations, thus hardening future slip systems. Self-hardening is accomplished by evolution of the subgrain structure length scale. The substructure length scale is computed by minimizing the nonlocal energy. The minimization of the nonlocal energy is a competition between the dislocation wall and boundary layer energy. The nonlocal terms are also directly minimized within

the subgrain model as they impact deformation response. The geometrical relationship between the dislocation walls and slip planes affecting dislocation mean that free path is accounted for, giving a first-order approximation to shape effects. A coplanar slip model is developed due to requirements when modeling the subgrain structure. This subgrain structure plasticity model is noteworthy as all material parameters are experimentally determined, rather than fit. The model also has an inherit path dependency due to the formation of the subgrain structures. Validation is accomplished by comparison with single crystal tension test results.

Evolution of the width between dislocation

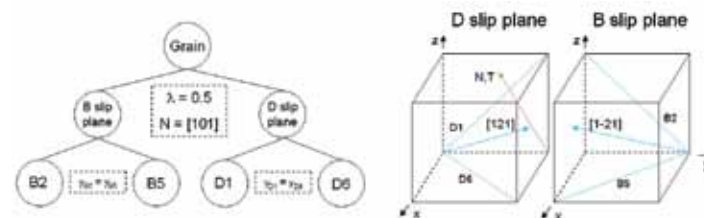


Fig. 2. The subgrain structure formed during the [101] simulation and the active slip systems in the crystallographic coordinates are given.

wall subgrain structures provides hardening mechanisms akin to those of self and latent hardening. The dimensions of the subgrain structure are determined by minimizing the nonlocal energy. The widths are equilibrated at each deformation step. Self-hardening occurs as the laminate width decreases due to increasing boundary layer energy of the laminate microstructure with increased deformation. The crystal bifurcating into separate regions to accommodate activation of new slip systems causes latent hardening to occur. The hardening behavior was validated against experimental tests of single crystal copper. Figure 1 shows a comparison between simulated and experimental stress-strain curves for copper single crystals. Three different crystal alignments are shown: [001], [101], and [102]. The crystal direction is aligned to the tensile axis. The single points are the experimental data from Franciosi (1985) [1]; the lines are computer simulations using the laminate hardening model. Note that there are two sets of experimental data for each crystal orientation. The simulations provide good validation for the hardening mechanisms of the model for these highly symmetric crystal orientations.

The subgrain structure formed during the [101] simulation and the active slip systems in the crystallographic coordinates are given in Fig. 2. The [101] orientation forms a simple laminate involving the B2 and B5 slip systems and the D1 and D6 slip systems.

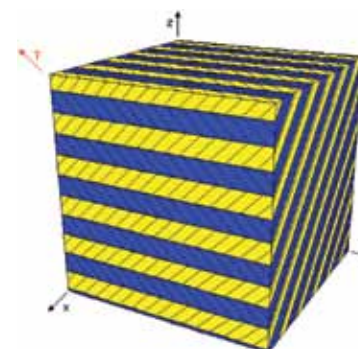


Fig. 3. Laminate formation

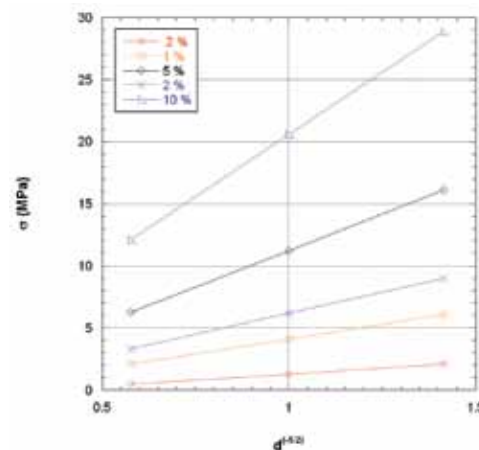


Fig. 4. Yield strengths

The black planes within the colored regions show the orientation of the active slip plane. The tensile axis, T, is included for reference.

All four active slip systems have the same strain level. The stress state of the sample has no shear stresses that would provide driving force for activation of further slip systems. The only nonzero stress in the simulation is the P33 component. Calculation of the Schmidt factor for the [101] orientation confirms that the four predicted slip systems have the highest Schmidt factor and should activate first. This is in agreement with Kalidindi and Amand [2], in which a traditional single crystal model was compared to a [101] copper single crystal deformed in compression. Kalidindi and Anand [2] also predicted that the same four slip systems would activate with equal strains. The deformation involves a shortening of the sample 2 direction (y in crystallographic coordinate system), while the 3 direction (or tensile axis, T, in the crystallographic coordinates) is elongated, and the 1 direction does not change. This same pattern of deformation is also seen in [2] with the experimental copper [101]-oriented compression sample. The trends are reversed due to the sample being in compression instead of tension (i.e., the 2 direction lengthens, while the 3 direction is compressed, and the 1 direction does not change in length). The agreement with deformed shape provides further evidence that the slip systems are correctly predicted. The stress response, activated

The dislocation wall normal, N, is parallel to the tensile axis, T – meaning the laminates form perpendicular to the tensile direction. A visualization of this structure in the crystal coordinates is given in Fig. 3 with color representing the regions in which the two different slip planes are active.

slip planes, and deformed shape are in excellent agreement with experimental data.

Figure 4 shows the yield strength of the [102] crystal response against the inverse of the square root of the initial grain size computed at various offset strains to the linear elastic deformation. The Hall-Petch relationship holds as the plots are linear. This relationship holds as long as a single layer of laminate forms, as was the case in all experiments examined here. It should also hold for higher-order laminate structures, except during the time steps in which the new laminates form. Uchic [3] and Greer [4] have recent work on the deformation response of micron-sized columns of single crystals. Their work showed that single crystals exhibit a Hall-Petch relationship, despite Hall-Petch having been found for polycrystals. The theory presented here shows the Hall-Petch effect due to the formation of dislocation subgrain structure with a grain size dependency, hence it provides a possible explanation for the Hall-Petch effect for both single crystals and polycrystals. Both Uchic[3] and Greer [4] also predicted a transition as sample size decreased to a breakaway flow behavior. This laminate theory would predict that transition as the length scale at which the deformation process no longer favors the formation of dislocation structures, but instead favors activation of a single slip system. The Uchic [3] experimental data is on a Ni₃Al-Ta alloy and the Greer [4] data is on gold, so no direct comparison is possible for the copper considered here. Thus, the theory presented here should follow the same trends discovered on micron-sized single crystals.

The results of simulations varying the grain shape are shown in Fig. 5. As this grain shape effect is due to the formation of subgrain structures inside the single crystal, rather than compatibility constraints within a polycrystalline sample, comparison would need to be made to similarly shaped single crystal tests. As of yet, no information is apparent for comparisons.

The model here contains only seven material parameters. All material parameters were measured directly by independent experimentation. It is

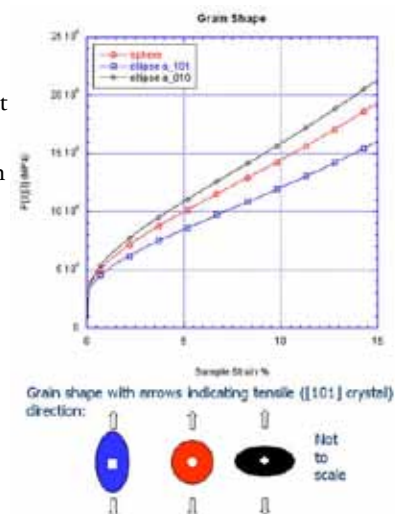


Fig. 5.

remarkable that the stress strain response can be predicted so well by the model with no fitting parameters.

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